# Universal Relation Connecting Fermi Surface to Symmetry of the Gap Function in BCS-Like Superconductors

Gang Su* and Masuo Suzuki†

*Department of Applied Physics, Faculty of Science, Science University of Tokyo*

*1-3, Kagurazaka, Shinjuku-ku, Tokyo 162, Japan*

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## Abstract

A universal relation connecting Fermi surface (FS) to the symmetry of the gap function in BCS-like superconductors is derived. It is found that the shape of the FS can be deduced directly from the symmetry of the superconducting gap function, and is also influenced by the next nearest-neighbor overlapping. The application of this relation to cuprate superconductors is discussed. There is observed an interesting property that Luttinger's theorem perfectly holds for the tight-binding band while it is violated by inclusion of the next nearest-neighbor overlapping integral.

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A number of recent experiments [1–4] on underdoped bilayer cuprate superconductors reveal that there appears a gap characterized by a large suppression of low frequency (spin and electronic) spectral weight near $(0, \pi)$ in the normal state. This unusual phenomenon is commonly referred to as the pseudogap (or spin gap, see, e.g. Refs. [5,6] for a review). Several scenarios, e.g. SU(2) gauge theory [7], spinon pairing [8], pairing correlations [9], superconducting (SC) fluctuations [10] and so on, are thereby proposed to explain this unusual phenomenon. In most of these theories, the Fermi surface (FS) plays a great role. The interest in studying theories of the FS is thus renewed. The question how the FS is related to the symmetry of the SC gap function, namely a basic issue for addressing the cause of the pseudogap phenomenon in our opinion, is still not quite clear and calls for explorations. Once we obtain the knowledge about the FS at zero temperature, we can study the temperature evolution [11] of the FS from this surface.

According to Luttinger [12], the FS can be defined as the locus in momentum space where the renormalized single-particle energy is equal to the chemical potential at zero temperature. In other words, if we know the zero-temperature chemical potential of the system, we know the shape of the FS. For superconductors when we lower the temperature down to zero, the system goes into the SC ground state. Considering that superconductivity develops directly from a metal, one may expect that the FS might have a close relation to the symmetry of the SC gap function. Since the symmetry of the SC gap function, e.g. in cuprate superconductors, can be clearly detected in experiments, it might offer us an opportunity to address the aforementioned question. Along this line, we shall write down in the present paper the general BCS-like SC ground-state wave function in which the gap function and the chemical potential are explicitly included. On account of it, a universal relation between the Fermi energy and the symmetry of the SC gap function can be obtained. When comparing it with cuprate superconductors, one could in turn gain insight into the structure of the SC ground state of cuprates. Generally speaking, for a given system the FS is also given, and by incorporating the given Hamiltonian one can determine the SC gap function from this FS. Our logic here is, however, inverse. In spite of the reasons above mentioned, our motivation also comes from the following two aspects. First, there is, at present, no consensus on the model Hamiltonian for cuprate superconductors, and meanwhile the controversial conclusions have been usually drawn in literature owing to the use of different Hamiltonians. In order to get reliable consequences in this situation, an alternative starting point might be Hamiltonian-free. Yet, the structure of the SC ground state would be the same, as detected in experiments, no matter what kind of Hamiltonians are assumed. Even if one is able to write down a Hamiltonian proper for cuprates, it is also not possible to obtain the exact SC ground state owing to complexity of many-body problems, like the celebrated BCS theory [13] in which the proposed wave function is neither an exact ground state nor an eigenstate of the electron-phonon interacting Hamiltonian. In fact, many people have used BCS-like schemes to construct their models for cuprate superconductors. Second, since the SC gap function in cuprates is already known, while the shape of the FS is now actively under debate, it appears possible to get some information of the FS directly from the gap function. Furthermore, one can use the obtained results to compare with experiments to examine whether the SC ground states of cuprates are of BCS-like form or not.

*SC wave function.* — It has been well established from the experiments like flux quantiza-

tion, Andreev reflection, Josephson effect, etc. that electrons responsible for superconductivity in cuprates are paired in singlet spin states (see, e.g. Ref. [14]), although the mechanism leading to electron pairing is still quite controversial. Therefore, the SC state can be considered as the condensation of these singlet electron pairs, implying that the corresponding SC wave function would be some kind of coherent superpositions of electron pairs. In addition, a number of measurements showed that the pairing symmetry in cuprates, namely the SC gap function over the FS, is anisotropic and has the $d_{x^2-y^2}$-wave character, demanding that any promising SC wave function should reflect this property. Considering the remarkable fact that the most successful pairing wave function up to date is BCS-like [13], we can first assume that the SC state of cuprate superconductors could also have a form similar to the BCS state, and then we observe if it is really so. The following discussion is based on this viewpoint. Before presenting our result, let us first give some preliminary definitions. The singlet electron pairing operator $b^\dagger_{\mathbf{k}}$ can be generally expressed in momentum space as

$$b^\dagger_{\mathbf{k}} = c^\dagger_{\mathbf{k}+\mathbf{Q}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}, \tag{1}$$

where $c^\dagger_{\mathbf{k}\uparrow}$ denotes the creation operator of a spin-up electron with momentum $\mathbf{k}$, and $\mathbf{Q}$ is the total momentum of an electron pair. The SC gap function is usually defined as

$$\Delta_{\mathbf{k}} = g(\mathbf{k})\Delta_0, \quad \Delta_0 = \langle b^\dagger_{\mathbf{k}} \rangle, \tag{2}$$

where $g(\mathbf{k})$ characterizes the pairing symmetry. The amplitude of the gap function, $\Delta_0$, depends generally on $\mathbf{k}$ and the doping parameter $\delta$, and can be in principle calculated explicitly from a given Hamiltonian. In most cases, $\Delta_0$ is often assumed to be $\mathbf{k}$ independent, like the SU(2) gauge theory developed in Refs. [7]. Equation (2) comprises the following cases. (1) Cooper pairing ($s$-wave): $g_s(\mathbf{k}) = 1$ and $\mathbf{Q} = (0, \cdots)$; (2) $\eta$ pairing: $g_\eta(\mathbf{k}) = 1$ and $\mathbf{Q} = (\pi, \cdots)$; (3) Extended $s$-wave pairing: $g_{e-s}(\mathbf{k}) = \cos k_x + \cos k_y$ and $\mathbf{Q} = (0, \cdots)$; (4) $d_{x^2-y^2}$-wave pairing: $g_{d_{x^2-y^2}}(\mathbf{k}) = \cos k_x - \cos k_y$ and $\mathbf{Q} = (0, \cdots)$; (5) $d_{xy}$-wave pairing: $g_{d_{xy}}(\mathbf{k}) = \sin k_x \sin k_y$ and $\mathbf{Q} = (0, \cdots)$; and so forth. For the $d_{x^2-y^2} + is$ ( $d_{x^2-y^2} + id_{xy}$)-wave mixing state, the SC gap function can be written as $\Delta_{\mathbf{k}} = \Delta_{d_{x^2-y^2}}(\mathbf{k}) + i\varepsilon\Delta_{s(d_{xy})}(\mathbf{k})$ with $\varepsilon$ the fraction of $s(d_{xy})$ component mixed with the $d_{x^2-y^2}$ state (see e.g. Ref. [15]). Hence, almost all currently interesting pairing scenarios are covered by this definition. With these definitions in mind, we now write down the general BCS-like SC wave function as the following form:

$$|\Psi_G\rangle = A_0 \exp(\sum_{\mathbf{k}} \xi(\{\mathbf{k}\}) c^\dagger_{\mathbf{k}+\mathbf{Q}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})|0\rangle, \tag{3}$$

where the variable $\xi(\{\mathbf{k}\})$ will be specified below, $|0\rangle$ is the vacuum satisfying $c_{\mathbf{k}\uparrow}(c_{\mathbf{k}\downarrow})|0\rangle = 0$, and $A_0$ is a normalization factor given by

$$A_0 = \frac{1}{\sqrt{\prod_{\mathbf{k}}(1 + |\xi(\{\mathbf{k}\})|^2)}}. \tag{4}$$

This form is quite natural, because Eq.(3) is nothing but a coherent state of the electron pairs, and breaks the U(1) symmetry. Considering the hard-core property of the pairing operator $b^\dagger_{\mathbf{k}}$, namely, $(b^\dagger_{\mathbf{k}})^2 = 0$, one may find that $|\Psi_G\rangle$ recovers the BCS form. We note

that some forms similar to Eq. (3) have been discussed in a few textbooks, but the gap symmetry and the pairing momentum are not particularly emphasized. However, the present form is more general, because it includes almost all pairing mechanisms with various pairing symmetries [16]. It turns out that Eq. (3) can serve as a reasonable variational wave function for the SC ground state. We would like to point out that unlike the RVB wave function [17] where the doubly-occupied sites are projected out owing to the assumption of the t-J model, we here do not necessarily do so, like the conventional BCS theory, as we consider the problem directly in momentum space and need not invoke *a priori* assumption of a large on-site Coulomb repulsion, which is also consistent with the definition of off-diagonal long-range order (ODLRO) in which the ODLRO on off-site pairing is strictly ruled out [18]. Besides, since the type-II superconductors (e.g. cuprate superconductors) are anisotropic, there are vortex cores existing in the range between the lower and the upper critical fields, suggesting that the equation (3) when applied to this case, might not work. However, we suppose that Eq.(3) would be universal in the absence of an applied field. [Above the lower but below the upper critical field, Eq. (3) might have other forms.] In general, $\xi(\{\mathbf{k}\})$ is a functional of the single-particle bare dispersion $\epsilon_{\mathbf{k}}$, the chemical potential $\mu$, the gap function $\Delta_{\mathbf{k}}$ and the doping parameter $\delta$:

$$\xi(\{\mathbf{k}\}) = \xi(\epsilon_{\mathbf{k}}, \mu, \Delta_{\mathbf{k}}, \delta), \tag{5}$$

where the $\delta$-dependence of $\xi(\{\mathbf{k}\})$ stemms from $\Delta_0$. If the Hamiltonian of the system is given, $\xi(\{\mathbf{k}\})$ can be in principle determined variationally. When applying Eq.(3) to Eq.(2) we get the following self-consistent equation

$$\Delta_{\mathbf{k}} = \frac{g(\mathbf{k})\xi(\{\mathbf{k}\})}{1+|\xi(\{\mathbf{k}\})|^2}. \tag{6}$$

This equation shows that the SC gap function is relevant to the chemical potential, i.e., the FS. Obviously, if we know an explicit form of $\xi(\{\mathbf{k}\})$, then we can gain some information on the FS.

*Fermi Surface.* — For the aim above mentioned, we may assume that $\xi(\{\mathbf{k}\})$ takes the following simplest form, i.e., the BCS-like form:

$$\xi(\{\mathbf{k}\}) = \frac{\Delta_{\mathbf{k}}}{\epsilon_{\mathbf{k}} - \mu + \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + |\Delta_{\mathbf{k}}|^2}}, \tag{7}$$

where we have scaled all the relevant energies with the overlapping integral $t$ which was taken to be unity. It should be noticed that any BCS-like mean-field theory in the weak-coupling ($\sim t$) limit can lead to the universal form of $\xi(\{\mathbf{k}\})$ like Eq. (7). Incorporating Eqs.(6) and (7), it gives rise to

$$\mu = \epsilon_{\mathbf{k}} - g(\mathbf{k})\sqrt{\frac{1}{4} - |\Delta_0|^2}. \tag{8}$$

For a mixing state like $d_{x^2-y^2} + is$ or $d_{x^2-y^2} + id_{xy}$, a similar calculation yields $\mu = \epsilon_{\mathbf{k}} - \tilde{g}(\mathbf{k})\sqrt{\frac{1}{4} - |\Delta_0|^2}$ with $\tilde{g}(\mathbf{k}) = \sqrt{g_{d_{x^2-y^2}}(\mathbf{k})^2 + \varepsilon^2 g_{s(d_{xy})}(\mathbf{k})^2}$. From Eq.(6) we know $|\Delta_0| \leq 1/2$, suggesting that the property for Eq. (8) to be real is guaranteed. Equation (8) shows

that the zero-temperature chemical potential (i.e., the Fermi energy), thereby the FS, is closely related to the symmetry of the gap function $g(\mathbf{k})$, except $|\Delta_0| = 1/2$ where the term containing the gap symmetry vanishes. This is subtle. At a first glance, this seems to be impossible, because the existence of the SC gap leads to that the FS has no definition in the SC state. However, one should not forget that superconductivity derives from a metal, and those electrons which are close to the FS of the metal are paired and responsible for superconductivity, while the chemical potential enters into the formalism as a constant, we therefore have Eq.(8). In other words, *the FS determined by Eq. (8) should be understood as that of the metal from which superconductivity develops.* One may observe that for the BCS theory, $g(\mathbf{k}) = 1$, the second term of Eq. (8) is a constant, showing that the shape of the FS is not affected by the SC gap, and is mainly controlled by the single-particle dispersion, as it should be. While for cuprate superconductors, the gap symmetry may be the $d_{x^2-y^2}$-wave. If the SC state can be written as the form of Eq. (3), then the shape of the FS may be obtained directly from Eq. (8). Experimentally, the single-particle dispersion for cuprates has the form

$$\epsilon_{\mathbf{k}} = -2(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y, \tag{9}$$

where we have taken $t = 1$ as an energy scale for simplicity. Typically, $t' = -0.05$ for LSCO and $-0.25$ for YBCO [19]. When we insert these data into Eq. (8), we find that the shape of the FS for LSCO is qualitatively different from that of experiments, while the FS for YBCO looks quite similar to the ARPES determined one in optimal doping. (Here we have assumed the $d_{x^2-y^2}$ symmetry and $|\Delta_0| = 0.07$ which comes from the experimental data $t \approx 0.5eV$ and $\Delta_0 \approx 35meV$ in both cases.) This implies that the structure of the SC ground state for LSCO could be different from that for YBCO, while the latter might be more similar to BCS-like one.

Now let us discuss which parameter affects primarily the shape of the FS. Equation (8) contains three parameters, namely $t'$, $\Delta_0$ and $g(\mathbf{k})$. For different values of $t'$, we find that the shapes of FS change drastically, as depicted in Fig. 1(a), where we have taken $t' = -1/4, -1/8, 0, 1/8, 1/4$ with $\Delta_0 = 0.07$ and $g(\mathbf{k}) = \cos k_x - \cos k_y$. It can be seen that the shape of the FS is gradually closed from $t' \leq 0$ (open) to $t' > 0$. In Fig. 1(b), we show contours for different values of $\Delta_0(= 0, 0.1, 0.2, 0.3, 0.4, 0.5)$ with $t' = -0.25$ and $g(\mathbf{k}) = \cos k_x - \cos k_y$. One can find that $\Delta_0$ does not play an important role in determining the shape of the FS. Since the doping dependence of $\Delta_{\mathbf{k}}$ comes only from $\Delta_0$, the present result shows that the doping does not have a significant effect on the shape of the FS in BCS-like superconductors, in sharp constrast to the experimental observations in cuprate superconductors where the evolution of the FS with the doping is clearly observed. This may imply that the BCS-like SC state could not be applied to the *whole* doping regime in cuprates, but this does not rule out the possibility that the BCS-like SC state can be applied to the cuprates in certain fixed doping regime. We also present the shapes of the FS for different gap symmetries with $t' = 0$, $\Delta_0 = 0.07$ and $\varepsilon = 0.3$, as shown in Fig. 2. We find that the FS for the s-wave and extended s-wave symmetries are the same (contour a). The reason is quite simple. For the s-wave symmetry, the second term of Eq. (8) is a constant, while for the extended s-wave symmetry that second term can be merged into the first term, leading to the same shape of the FS as that of the s-wave. The FS for the $d_{x^2-y^2}$-wave symmetry is open, and composed of two separated cosine-like curves (contours b), while for

the $d_{xy}$-wave symmetry the FS looks like a slightly deformed and closed square (contour c). For a mixing state $d_{x^2-y^2} + id_{xy}$, we see that the FS consists of four arcs (contours d), similar to (but not the same as) the FS for the $d_{x^2-y^2}$-wave symmetry with $t' = -0.25$. This demonstrates that the FS for the d-wave symmetry differs from that for the s-wave, while it makes us not easy to identify which state, the $d_{x^2-y^2}$ with next nearest-neighbor overlapping or the $d_{x^2-y^2} + id_{xy}$ with only tight-binding band, is more suitable for cuprates like YBCO or BSCCO. Nonetheless, we could remark that the shape of the FS in BCS-like superconductors can be deduced directly from the symmetry of the SC gap function, and is also influenced by the magnitude of the next nearest-neighbor overlapping integral $t'$.

*Luttinger's Theorem.* — Almost forty years ago on the basis of an adiabatically perturbative expansion, Luttinger was able to show that the volume (or area in two dimensions) enclosed by the FS for interacting electrons is the same as that for noninteracting electrons [12], the assertion now known as Luttinger's theorem. Later on, people find that this theorem indeed holds in most cases, but exceptions were also found particularly in strongly correlated electrons, where it was shown that this theorem was violated (see e.g. Refs. [20]). How about Luttinger's theorem in BCS-like superconductors? In accordance with Eq. (8), we draw the FS for the noninteracting and interacting cases, as shown in Fig. 3(a), where we have taken $t' = 0$, $\Delta_0 = 0.07$ and $g(\mathbf{k}) = \cos k_x - \cos k_y$. (Note that in this case the FS for the noninteracting system is a square.) After carefully checking the areas enclosed by two surfaces, we find that the two areas enclosed by the FS are exactly the same. We also checked other values of $\Delta_0$ for different gap symmetries but keep $t' = 0$, and the same result was observed, namely, Luttinger's theorem perfectly holds in this case. When we increase the magnitude of the next nearest-neighbor overlapping $t'$, we find that Luttinger's theorem becomes violated, even for a slight tuning-on of $t'$. Shown in Fig. 3(b) is for $t' = -0.05$, $\Delta_0 = 0.07$ and $g(\mathbf{k}) = \cos k_x - \cos k_y$. From this figure, one can see that the areas enclosed by the two surfaces are not equal, i.e., the area enclosed by the FS (i.e. four arcs) for the noninteracting system is larger than that for the interacting system. The present result reveals that the inclusion of next nearest-neighbor overlapping integral, a property of strongly correlated electrons, will violate Luttinger's theorem, no matter what kind of gap symmetries (except the s-wave) are used, implying no adiabatic connection between interacting and noninteracting systems in this case. Therefore, the present result is compatible with the statement in Refs. [20], i.e., strong correlations between electrons might violate Luttinger's theorem.

In summary, we have derived a universal relation connecting the Fermi surface to the gap symmetry in BCS-like superconductors. On the basis of it, we showed that the shape of the FS in BCS-like superconductors can be deduced directly from the symmetry of the SC gap function, and is affected by the next nearest-neighbor overlapping integral. When this universal relation applied to cuprate superconductors, we found that the BCS-like SC state with $d_{x^2-y^2}$-wave symmetry could not be suited to LSCO, while it is probably applicable to YBCO and BSCCO. Finally, we observed that Luttinger's theorem perfectly holds for the tight-binding band, while the inclusion of next nearest-neighbor overlapping would violate this theorem, which is consistent with some previous investigations in strongly correlated electrons. Although our derivation is quite simple, the result in our opinion contains essential physical consequences. We expect that our presentation could offer some bases for understanding the pseudogap phenomenon and the temperature evolution of the Fermi

surface in cuprate superconductors.

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*On leave from Graduate School, Chinese Academy of Sciences, Beijing, China. Electronic address: gsu@ap.kagu.sut.ac.jp

†Electronic address: msuzuki@ap.kagu.sut.ac.jp

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## FIGURES

Fig.1 The evolution of the Fermi surfaces with: (a) next nearest-neighbor overlapping integral $t'(= -1/4, -1/8, 0, 1/8, 1/4)$ with $|\Delta_0| = 0.07$; (b) the amplitude of the SC gap function $|\Delta_0|(= 0, 0.1, 0.2, 0.3, 0.4, 0.5)$ with $t' = -0.25$. In both cases, $g(\mathbf{k}) = \cos k_x - \cos k_y$.

Fig.2 The shapes of the Fermi surface for different symmetries of the SC gap function. Contour a: s-wave and extended s-wave; b: $d_{x^2-y^2}$-wave; c: $d_{xy}$-wave; d: $d_{x^2-y^2} + id_{xy}$-wave. Here $t' = 0$, $|\Delta_0| = 0.07$ and $\varepsilon = 0.3$.

Fig.3 Illustration of Luttinger's theorem (see text). (a) $t' = 0$; (b) $t' = -0.05$. In both cases, $|\Delta_0| = 0.07$ and $g(\mathbf{k}) = \cos k_x - \cos k_y$.